

(FILE 'HOME' ENTERED AT 16:11:16 ON 21 MAR 2006)

L1 FILE 'CAPLUS' ENTERED AT 16:11:28 ON 21 MAR 2006
STRUCTURE uploaded
S L1

L2 FILE 'REGISTRY' ENTERED AT 16:11:49 ON 21 MAR 2006
27 S L1

L3 FILE 'CAPLUS' ENTERED AT 16:11:50 ON 21 MAR 2006
12 S L2

L4 7 S L3 AND PY<1997

L5 STRUCTURE uploaded
S L5

L6 FILE 'REGISTRY' ENTERED AT 16:18:54 ON 21 MAR 2006
0 S L5

L7 FILE 'CAPLUS' ENTERED AT 16:18:55 ON 21 MAR 2006
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L8 STRUCTURE uploaded
S L8

L9 FILE 'REGISTRY' ENTERED AT 16:21:30 ON 21 MAR 2006
109 S L8 SSS FULL

L10 FILE 'CAPLUS' ENTERED AT 16:22:01 ON 21 MAR 2006
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L11 28 S L10 AND PY<1997

L12 FILE 'CAPLUS' ENTERED AT 16:39:52 ON 21 MAR 2006
STRUCTURE uploaded
S L12

L13 FILE 'REGISTRY' ENTERED AT 16:40:18 ON 21 MAR 2006
2 S L12

L14 FILE 'CAPLUS' ENTERED AT 16:40:19 ON 21 MAR 2006
2 S L13
S L12

L15 FILE 'REGISTRY' ENTERED AT 16:41:18 ON 21 MAR 2006
194 S L12 SSS FULL

L16 FILE 'CAPLUS' ENTERED AT 16:41:19 ON 21 MAR 2006
360 S L15 SSS FULL

L17 287 S L16 AND PY<1997

L18 10 S L17 AND F AND CL

L19 STRUCTURE uploaded

L20 STRUCTURE uploaded
S L20

L21 FILE 'REGISTRY' ENTERED AT 16:48:37 ON 21 MAR 2006
0 S L20

L22 FILE 'CAPLUS' ENTERED AT 16:48:39 ON 21 MAR 2006
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S L20

L23 FILE 'REGISTRY' ENTERED AT 16:48:48 ON 21 MAR 2006
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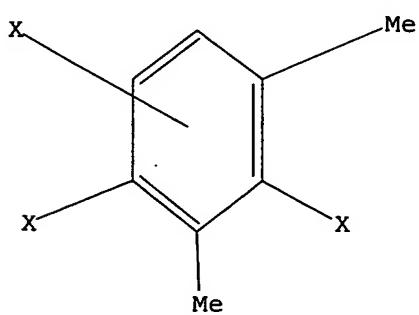
L24 FILE 'CAPLUS' ENTERED AT 16:48:49 ON 21 MAR 2006
1 S L23 SSS FULL

L19 : STRUCTURE UPLOADED

=> d

L19 HAS NO ANSWERS

L19 STR



Structure attributes must be viewed using STN Express query preparation.

=> d 1-10 ibib abs hitstr

L24 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:709043 CAPLUS

DOCUMENT NUMBER: 129:316044

TITLE: 3-Cyano-2,4,5-trifluorobenzoyl fluoride and
intermediates for its production

INVENTOR(S): Marhold, Albrecht; Wolfrum, Peter

PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

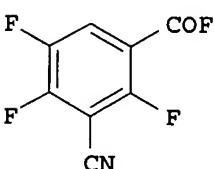
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9847862	A1	19981029	WO 1998-EP2175	19980414
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE 19717231	A1	19981029	DE 1997-19717231	19970424
CA 2287176	AA	19981029	CA 1998-2287176	19980414
AU 9872163	A1	19981113	AU 1998-72163	19980414
EP 977729	A1	20000209	EP 1998-919266	19980414
EP 977729	B1	20020313		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
JP 2001521534	T2	20011106	JP 1998-544950	19980414
AT 214365	E	20020315	AT 1998-919266	19980414
ES 2174431	T3	20021101	ES 1998-919266	19980414
CN 1119324	B	20030827	CN 1998-804339	19980414
IL 131974	A1	20040219	IL 1998-131974	19980414
US 6229040	B1	20010508	US 1999-403263	19991015
HK 1027555	A1	20040514	HK 2000-106792	20001025
US 2001023300	A1	20010920	US 2001-814132	20010321
US 6541675	B2	20030401		
US 2003092929	A1	20030515	US 2002-277310	20021022
US 6706918	B2	20040316		
CN 1436771	A	20030820	CN 2002-148153	20021031
US 2004167350	A1	20040826	US 2003-749593	20031231
PRIORITY APPLN. INFO.:			DE 1997-19717231	A 19970424
			WO 1998-EP2175	W 19980414
			US 1999-403263	A3 19991015
			US 2001-814132	A1 20010321
			US 2002-227310	A3 20020826

GI



I

AB 3-Cyano-2,4,5-trifluorobenzoyl fluoride (I) is prepared starting from 5-fluoro-m-xylene and proceeding via 2,4-dichloro-5-fluoro-1,3-dimethylbenzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)-1-(trichloromethyl)benzene, 2,4-dichloro-5-fluoro-3-(dichloromethyl)benzoic acid, 2,4-dichloro-5-fluoro-3-formylbenzoic acid (II), the oxime of II,

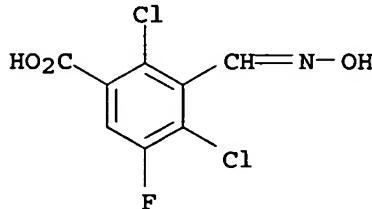
IT and 2,4-dichloro-3-cyano-5-fluorobenzoyl chloride.

214774-57-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination-dehydration of)

RN 214774-57-9 CAPLUS

CN Benzoic acid, 2,4-dichloro-5-fluoro-3-[(hydroxyimino)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 118 1-10 ibib abs hitstr

L18 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:428577 CAPLUS

DOCUMENT NUMBER: 115:28577

TITLE: Formation constants in carbon-hydrogen hydrogen bonding. 2. Alkynes and polyhalobenzenes with hexamethylphosphoric triamide in cyclohexane solution

AUTHOR(S): Lorand, John P.; Nelson, Jonathan P.; Gilman, R. Dean; Staley, Kathy L.; Chambers, Jeffery R.; Kirk, Harold D.; Moeggenborg, Kevin J.; Farlow, David L.

CORPORATE SOURCE: Dep. Chem., Cent. Michigan Univ., Mt. Pleasant, MI, 48859, USA

SOURCE: Journal of Physical Organic Chemistry (1990), 3(10), 659-69

CODEN: JPOCEE; ISSN: 0894-3230

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Formation consts., K, for hydrogen bonding of weak C-H donors with hexamethylphosphoric triamide were measured in cyclohexane at 35° by PMR, data were analyzed by the Higuchi method. Donors include terminal alkynes and polyfluoro-, polychloro-, and polybromobenzenes. The K values for many of these are too small to measure in CCl₄. For R-CH₂ > C₆H₅ > C₂H₅O > tert-Bu. For polyhalobenzenes, K is generally larger for F than Cl or Br, and meta halogens facilitate hydrogen bonding most effectively. Among tetrahalobenzenes, 1,2,3,4-isomers show the least evidence of 2:1 complex formation. Pentachlorobenzene has a smaller K than its 1,2,3,4-tetrachloro analog even after statistical correction; for C₆H₅X₅, K decreases in the order F > Cl > Br; the K values for 1,3,5-trihalobenzenes are closely similar; and 1,3,5-tribromo-2,4-dimethylbenzene shows no evidence of hydrogen bonding by PMR. The last three observations suggest that buttressing is important in the C₆H₅X₅ structure, at least with Cl and Br. A value of K for benzene was measured, suggesting for the first time that the H atoms of benzene engage in hydrogen bonding. The result compares well with values extrapolated from data for polyfluoro- but not polychlorobenzenes, again probably because of buttressing in the latter.

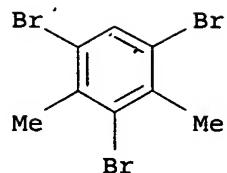
IT 134636-45-6P, 1,3,5-Tribromo-2,4-dimethylbenzene

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and attempted hydrogen bonding of, to HMPT in cyclohexane)

RN 134636-45-6 CAPLUS

CN Benzene, 1,3,5-tribromo-2,4-dimethyl- (9CI) (CA INDEX NAME)



L18 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1988:473266 CAPLUS

DOCUMENT NUMBER: 109:73266

TITLE: New manganese tetrakis(halogenoaryl)porphyrins featuring sterically hindering electronegative substituents: synthesis of highly stable catalysts in olefin epoxidation

AUTHOR(S): Banfi, Stefano; Montanari, Fernando; Quici, Silvio
CORPORATE SOURCE: Dip. Chim. Org. Ind., Univ. Milano, Milan, 20133, Italy

SOURCE: Journal of Organic Chemistry (1988), 53(12), 2863-6

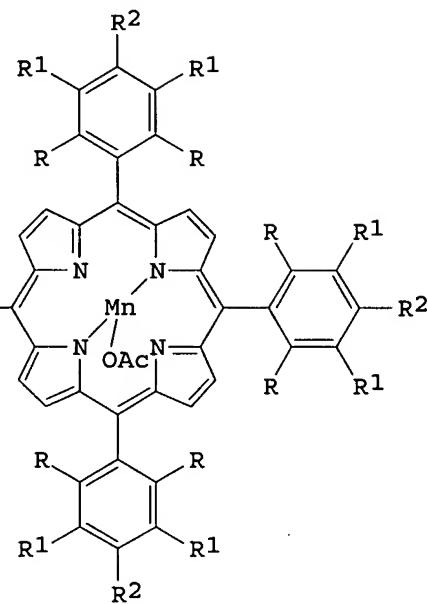
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 109:73266

GI



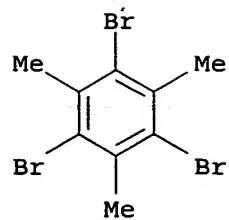
AB The complexes I ($R = R_2 = Cl$, Br , $R_1 = Me$; $R = R_2 = H$, $R_1 = Cl$) were prepared from halomesitylenes via condensation of halobenzaldehydes with pyrrole and complexation with $Mn(OAc)_2$. I ($R = Cl$, $R_1 = R_2 = H$; $R = R_2 = Cl$, Br , $R_1 = Me$) are highly stable and efficient catalysts for the epoxidn. of cyclooctene and 1-dodecene with $NaOCl$ at pH 9.5 and 0° under two-phase conditions, in the presence of N-hexylimidazole as axial ligand. The chemical stability dramatically decreases in I ($R=R_2 = H$, F ; $R = R_2 = Me$, $R_1 = H$; $R = R_2 = H$, $R_1 = Cl$).

IT 608-72-0, 2,4,6-Tribromomesitylene

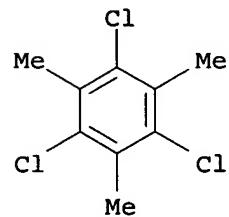
RL: RCT (Reactant); RACT (Reactant or reagent)
(conversion to dimethyltribromobenzyl alc.)

RN 608-72-0 CAPLUS

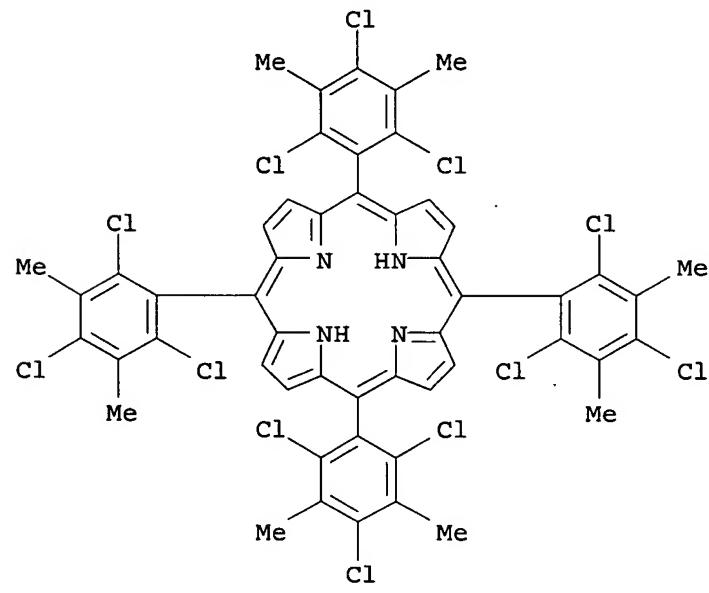
CN Benzene, 1,3,5-tribromo-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



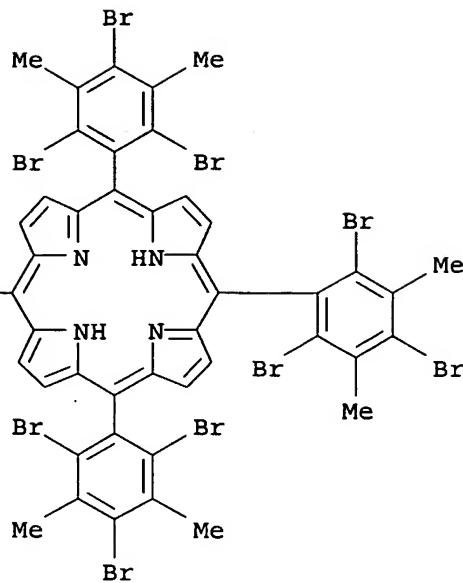
IT 5324-68-5, 2,4,6-Trichloromesitylene
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conversion to dimethyltrichlorobenzyl alc.)
 RN 5324-68-5 CAPLUS
 CN Benzene, 1,3,5-trichloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



IT 114634-36-5P 114634-37-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and complexation of, with manganese)
 RN 114634-36-5 CAPLUS
 CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,4,6-trichloro-3,5-dimethylphenyl)-
 (9CI) (CA INDEX NAME)



RN 114634-37-6 CAPLUS
 CN 21H,23H-Porphine, 5,10,15,20-tetrakis(2,4,6-tribromo-3,5-dimethylphenyl)-
 (9CI) (CA INDEX NAME)



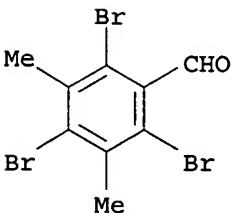
IT 114634-34-3P 114634-35-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and coupling of, with pyrrole)

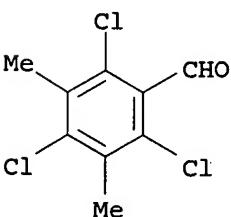
RN 114634-34-3 CAPLUS

CN Benzaldehyde, 2,4,6-tribromo-3,5-dimethyl- (9CI) (CA INDEX NAME)



RN 114634-35-4 CAPLUS

CN Benzaldehyde, 2,4,6-trichloro-3,5-dimethyl- (9CI) (CA INDEX NAME)



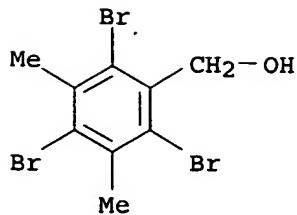
IT 114634-32-1P 114634-33-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

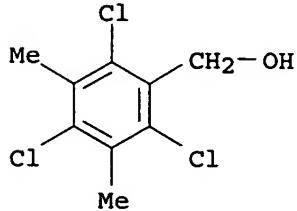
(preparation and oxidation of)

RN 114634-32-1 CAPLUS

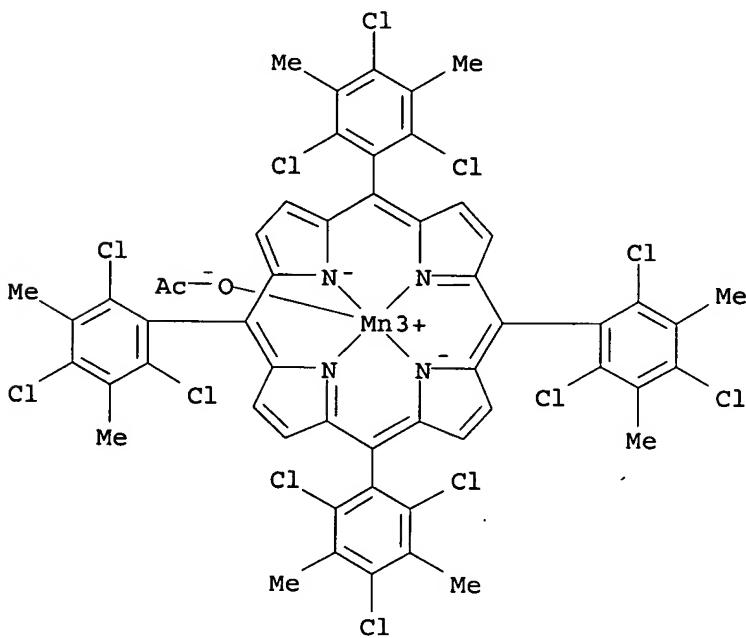
CN Benzenemethanol, 2,4,6-tribromo-3,5-dimethyl- (9CI) (CA INDEX NAME)



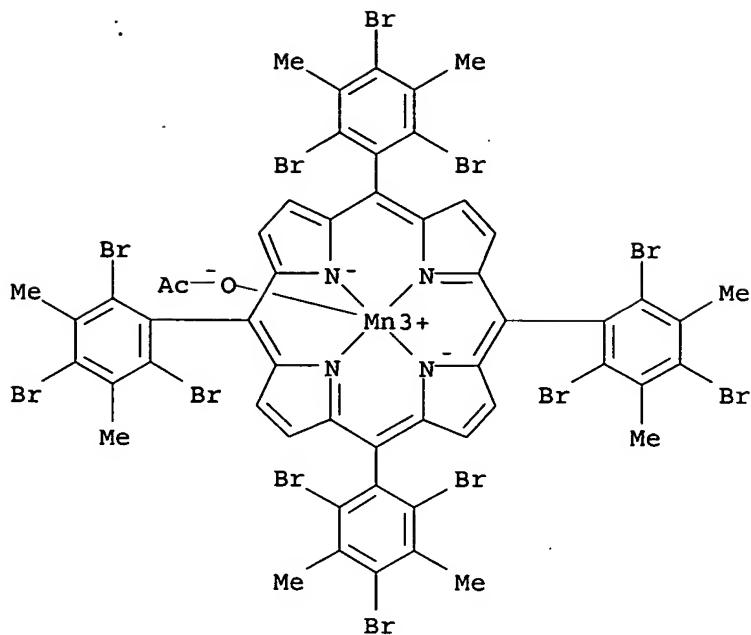
RN 114634-33-2 CAPLUS
 CN Benzenemethanol, 2,4,6-trichloro-3,5-dimethyl- (9CI) (CA INDEX NAME)



IT 114651-81-9P 114651-82-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as epoxidn. catalyst, stability of)
 RN 114651-81-9 CAPLUS
 CN Manganese, (acetato-O) [5,10,15,20-tetrakis(2,4,6-trichloro-3,5-dimethylphenyl)-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9CI)
 (CA INDEX NAME)



RN 114651-82-0 CAPLUS
 CN Manganese, (acetato-O) [5,10,15,20-tetrakis(2,4,6-tribromo-3,5-dimethylphenyl)-21H,23H-porphinato(2-)-N21,N22,N23,N24]-, (SP-5-12)- (9CI)
 (CA INDEX NAME)



L18 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1977:422689 CAPLUS

DOCUMENT NUMBER: 87:22689

TITLE: Permmercurated arenes. Part II. Synthesis of perbromobenzoic acids and perbromobenzenes from aromatic carboxylic acids by permmercuration and bromodemercuration

AUTHOR(S): Deacon, Glen B.; Farquharson, Graeme J.

CORPORATE SOURCE: Chem. Dep., Monash Univ., Clayton, Australia
SOURCE: Australian Journal of Chemistry (1977),

30(2), 293-303

CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal

LANGUAGE: English

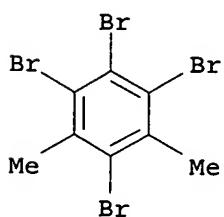
AB Mercuration of $RC_6H_4CO_2H$ ($R = 2\text{-Me, -Cl, -F, and -Br, 3\text{-Me, -F, -Cl, -Br, -CF}_3, -NO_2, and -OMe, and 4\text{-Me, -F, -Cl, -Br, -CF}_3, and -NO_2}$) and $2,6\text{-R}_2C_6H_3CO_2H$ ($R = \text{Me, Cl, Br}$) with $(CF_3CO_2)_2Hg$ and subsequent bromodemercuration gave the resp. $RC_6Br_4CO_2H$ and $2,6\text{-R}_2C_6Br_3CO_2H$, which were accompanied by C_6Br_5R and $1,3\text{-R}_2C_6Br_4$.

IT 39568-70-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 39568-70-2 CAPLUS

CN Benzene, 1,2,3,5-tetrabromo-4,6-dimethyl- (9CI) (CA INDEX NAME)



L18 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1976:179885 CAPLUS

DOCUMENT NUMBER: 84:179885

TITLE: Quality of phthalic acids improved by haloacetic acid
INVENTOR(S): Kuhlmann, George E.

PATENT ASSIGNEE(S): Standard Oil Co., USA

SOURCE: U.S., 6 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3947494	A	19760330	US 1972-316857	19721220 <--
			US 1972-316857	A 19721220

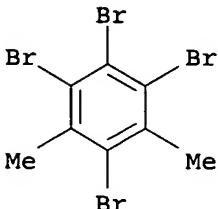
PRIORITY APPLN. INFO.: AB Phthalic acids of improved quality were obtained by direct oxidation of xylenes (e.g., o- and p-xylene, m- and p-Me₂C₆Br₄, p-Me₂C₆Cl₄) with O in an oxidation zone with small amts. of haloacetic acid, e.g., XCH₂CO₂H (X = Cl, Br, F) or F₃CCO₂H, present in HOAc solution of one or more heavy metal oxidation catalysts and Br-releasing Br-containing compound BrCH₂CO₂H was the most effective acid tested.

IT 39568-70-2

RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, effect of haloacetic acids on quality of phthalic acids from)

RN 39568-70-2 CAPLUS

CN Benzene, 1,2,3,5-tetrabromo-4,6-dimethyl- (9CI) (CA INDEX NAME)



L18 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1972:447779 CAPLUS

DOCUMENT NUMBER: 77:47779

TITLE: Stable carbocations. CXXXIX. Nitro- and chlorohexamethylbenzenium ions and 1-nitro- and 1-chloro-2,4,6-trifluoromesitylenium ions

AUTHOR(S): Olah, George A.; Lin, Henry C.; Mo, Y. K.

CORPORATE SOURCE: Dep. Chem., Case West. Reserve Univ., Cleveland, OH, USA

SOURCE: Journal of the American Chemical Society (1972), 94(10), 3667-9

DOCUMENT TYPE: CODEN: JACSAT; ISSN: 0002-7863

LANGUAGE: Journal

GI For diagram(s), see printed CA Issue.

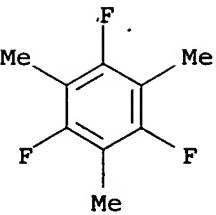
AB Hexamethylbenzeniums (I, X = NO₂, Cl) and 2,4,6-trifluoro-mesityleniums (II, X = NO₂, Cl) were obtained by treating Me₆C₆ or 1,3,5,2,4,6-F₃Me₃C₆ with NO₂+BF₄-FSO₃H-SO₂ and SbF₅-FSO₃H-Cl₂-SO₂ClF solution at low temperature. The structure of the ions were confirmed by PMR and F NMR. The PMR of I (R = NO₂) is temperature dependent indicating the degenerate migration or exchange process of the nitro group (NO₂⁺). The energy of activation of the process was 16.8 ± 1.5 kcal/mole.

IT 363-64-4

RL: PRP (Properties)
(benzenium ion formation from)

RN 363-64-4 CAPLUS

CN Benzene, 1,3,5-trifluoro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



L18 ANSWER 6 OF 10. CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1963:441438 CAPLUS

DOCUMENT NUMBER: 59:41438

ORIGINAL REFERENCE NO.: 59:7428d-h,7429a-c

TITLE: Perchloryl aromatic compounds

INVENTOR(S): Inman, Charles E.; Oesterling, Robert E.; Tyezkowski, Edward A.

PATENT ASSIGNEE(S): Pennsalt Chemicals Corp.

SOURCE: 12 pp.

DOCUMENT TYPE: Patent

LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3076853	-----	19630205	US 1962-204296	19620621 <--
			US	19620621

PRIORITY APPLN. INFO.:

AB The title compds. ArClO_3 were prepared by treating the appropriate aromatic compound with ClO_3F in the presence of a Freidel-Crafts catalyst. AlCl_3 was the preferred catalyst. An excess of the aromatic compound or an inert solvent may be used. Thus, AlCl_3 133 was suspended with agitation in benzene 2600 parts in a cooling bath. ClO_3F gas 100 patts was slowly passed into the mixture and the temperature maintained at 40° . Gaseous HCl was evolved. After HCl evolution had ceased, the reaction mass was added to twice its volume of H_2O , and steam-distilled. The benzene layer was evaporated and distilled in vacuo to give perchlorylbenzene 62 parts, b. 232° , f.p. -3° , n_{20}^D 1.5236, d_{30}^D 1.185. Similarly prepared were the following substituted perchlorylbenzenes [substituent(s) given]: 2,4-dimethyl; 2,5-dimethyl (b.p. 78° , m. $27-8^\circ$); 4-fluoro (b.p. 53°, n_{20}^D 1.5051); 2,5-dibromo; 2,5-dimethyl; 2,5-difluoro; 3,4-dimethyl; 4-hydroxy; 3,4-dibromo; 2,4-dimethyl; 2,5-dimethyl-4-chloro; 3,4,5-trichloro; 2,5-dichloro-3-fluoro; 2,4,6-trimethyl; 2,3,5,6-tetramethyl; 2-chloro-5-fluoro. A solution of perchlorylbenzene 20 in concentrated H_2SO_4 80 was treated with a mixture of concentrated H_2SO_4 25 and concentrated HNO_3 14 parts at 20-300 for 1 hr. The mixture was poured over ice and a yellow solid 22 parts was filtered from the mixture. Recrystn. from benzene-petr. ether gave yellow 3-nitroperchlorylbenzene, m. 49-50°, reduced with SnCl_2 in alc. HCl to 3-aminoperchlorylbenzene, m. 32°. The following substituted perchlorylbenzenes were prepared by known methods [substituent(s) given]: B-NH₂.HCl; 3-acetamido (m. 136 70); 4-Cl; 4-Me; 3,4-dichloro; 3-amino-4-methyl; 3-amino-4-methyl-6-nitro; 2,3,5-trichloro-4-fluoro; 2,3,5,6-tetrachloro-4-hydroxy-; 3-HO₃S; 2-MeO; 2-Cl; 2-chloro-5-nitro; 4-MeS; 3-(4-nitrophenyl); 4nitro-3-(4-nitrophenyl); 2-chloro-5-amino; 2-chloro-3-nitro-5amino; 2-Me; 3,5,6-trichloro-2-methyl; 3,4,5-trichloro-2-methyl; 2,3,4,5,6-pentachloro; 2,5-dimethyl-3-cyano; 3,4-dichloro-2,5difluoro; 3,6-dichloro-2,5-difluoro; 3,4-dichloro-5-methoxy; 3,4dichloro-5-phenyl; 3,4-dibromo-2,5-dichloro; 2,4-bis(chloromethyl); 2,4,5-trimethyl-3-nitro; 3,4,5-trichloro-2-iodo; 2,4,5,6-tetrachloro-3-fluoro; 3-iodo-2,4,6-trimethyl; 4-amino-2,3,5,6tetramethyl; 3-acetamido-2-nitro; 2,5-diamino-3-chloro; 3(3-perchlorylphenyl); 4-chloromethyl. Also prepared were azobis(3-perchlorylbenzene), azoxybis(3-perchlorylbenzene), and hydrazobis(3-perchlorylbenzene). 3-Aminoperchlorylbenzene-HCl 1 part was dissolved in 20% HCl and diazotized with NaNO_2 solution at 0-5° to form a solution of the diazonium salt. Yellow crystals of 3,3'-diperchloryldiazoaminobenzene were removed by filtration. To the

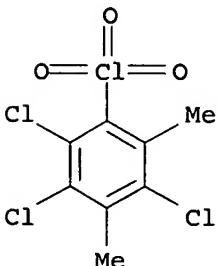
filtrate was added β -naphthol 1 part dissolved in dilute NaOH to give dark orange 3-(β -hydroxynaphthylazo)perchlorylbenzene, m. 200-1°. A mixture of 0.0233 mole 4-fluoroperchlorylbenzene and 0.221 mole NaOMe in 200 ml. MeOH was refluxed for 90 min., the cooled mixture diluted with H₂O, and extracted with Et₂5 to give 4-methoxyperchlorylbenzene, n_D0 1.5307. 4-Phenylthioperchlorylbenzene, n_D6 1.5778, was similarly prepared from 4-fluoroperchlorylbenzene and thiophenol in the presence of Na-OMe. 4-Chloroperchlorylbenzene was also prepared by chlorination of perchlorylbenzene at 10-16° in the presence of 1% anhydrous FeCl₃. Other nuclear chlorinated compds. were similarly prepared by continuing chlorination below 280° to substitution tip to 5 Cl atoms. Bromo- and iodoperchlorylbenzene compds. were similarly prepared using the appropriate halide catalyst (FeBr₃, iodine, or Fe). Alkylhaloperchloryl aryl compds. were prepared by halogenating the alkylperchloryl aryl compound. Thus, 2,4-dimethyl-perchlorylbenzene was progressively chlorinated, first at 5-10° and then by gradually raising the temperature to 60°, with gaseous Cl in the presence of FeCl₃ and in a suitable solvent (ClCH₂CCl₃, CCl₄, PhNO₂, Et₂O, EtOH, CHCl₃, or glacial HO₃c) to give 3-chloro-, 3,5-dichloro-, and 3,5,6-trichloro-2,4-dimethylperchloryl-benzene. Chlorination of 2,4-dimethylperchlorylbenzene was carried out in a glass tower packed with glass rings and illuminated with Hg lamps spaced 4 ft. apart. The 2,4-dimethyl-perchlorylbenzene was heated to 65-75° and red into the top of the tower at a uniform rate. Dry Cl gas was passed up the tower. The temperature of the tower was kept just below the reflux point and 2,4-chloromethylperchlorylbenzene was recovered as product. Highly alkylated and hydroxy-containing derivs. of perchloryl-benzene were chloromethylated by treating the perchloryl aryl compound with HCHO and HCl below 280° in the presence of H₂SO₄, ZnCl₂, Al, or Sn as catalysts. Perchlorylbenzene and its homologs were sulfonated by heating a mixture of the perchloryl aryl compound and concentrated H₂SO₄ below 280°. The title compds. were useful as explosives. 3-(β -Hydroxynaphthylazo)perchlorylbenzene was useful as a dye for wool.

IT 90048-78-5, m-Xylene, 2,4,5-trichloro-6-perchloryl-
90151-28-3, m-Xylene, 2,4-dichloro-6-perchloryl-

(preparation of)

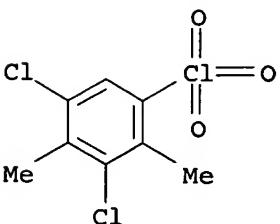
RN 90048-78-5 CAPLUS

CN m-Xylene, 2,4,5-trichloro-6-perchloryl- (7CI) (CA INDEX NAME)



RN 90151-28-3 CAPLUS

CN m-Xylene, 2,4-dichloro-6-perchloryl- (7CI) (CA INDEX NAME)



DOCUMENT NUMBER: 58:81229
 ORIGINAL REFERENCE NO.: 58:13841b-h
 TITLE: Perchloryl aromatic compounds
 INVENTOR(S): Inman, Charles E.; Oesterling, Robert E.; Tyezkowski, Edward A.
 PATENT ASSIGNEE(S): Pennsalt Chemicals Corp.
 SOURCE: 12 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3070609		19621225	US 1962-204295	19620621 <--
PRIORITY APPLN. INFO.:			US	19620621

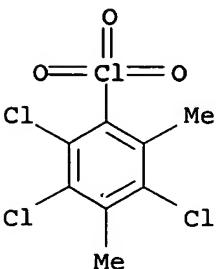
AB The F atom of FClO_3 (I) (perchloryl fluoride, b. -47.5°), was replaced with a substituted or unsubstituted aryl radical, by using a new organic unit process, perchlorylation (similarly to nitration, sulfonation, etc.), to form perchloryl aromatic compds. These can be further treated (sulfonated, halogenated, etc.). The new compds. possess explosive properties; they are useful as explosive charges for blasting and for the manufacture of explosive devices, also as high energy fuels, as intermediates in the preparation of compds. useful in pharmaceutical and dye application, as additives for fuels in internal combustion engines, particularly as cetane improvers in diesel fuels. To prepare these compds., I in gaseous form and the aromatic compound (preferably C_6H_6 , or substituted C_6H_6 as PhMe, PhEt, xylenes, mono-, di-, and trihalobenzenes; and chlorotoluenes) are brought together in stoichiometric proportions in the presence of Friedel-Crafts catalysts, as AlCl_3 , about mole per mole, in a nonalk., nonaq. system at $0-80^\circ$ (preferably $0-15^\circ$ for most of the reactions). Preferably, the catalyst is added to the aromatic compound, with the latter being used alone in excess or dissolved in a nonaq., inert solvent or diluent, and I is then passed into the mixture with agitation. The perchlorylated aromatic compds. can be treated under mildly alkaline, neutral, or acid conditions, below 280° around which temperature the ClO_3 group is unstable and the compds. decompose explosively. The ClO_3 group is replaced by HO group upon treatment with inorg. or organic base under strongly alkaline conditions. Thus, 133 parts AlCl_3 was suspended with agitation in 2600 parts C_6H_6 in a vessel in a cooling bath. I gas was passed slowly into the C_6H_6 - AlCl_3 mixture which was maintained at 40° . HCl gas was evolved from the reaction mass. Addition of I was stopped when 100 parts had been added and HCl evolution ceased. The reaction mass was added to twice its volume of water. The mass was then steam-distilled. The C_6H_6 layer thus recovered was evaporated, and the PhClO_3 contained therein, 70 parts, was recovered as a pale yellow oil. Distillation in vacuo gave 62 parts PhClO_3 , b. 282° f.p. -3° $n_{20D} 1.5236$, $d_{30} 1.186$. Similarly, from $m\text{-C}_6\text{H}_4(\text{CH}_3)_2$ (with AlCl_3 and I), $2,4\text{-Me}_2\text{C}_6\text{H}_3\text{ClO}_3$ was obtained, b. 78° . From PhF (with AlCl_2 and I), $4\text{-FC}_6\text{H}_4\text{ClO}_2$ was obtained, b. $0.25-53^\circ$, $n_{20D} 1.5051$. From $3\text{-O}_2\text{NC}_6\text{H}_4\text{ClO}_3$ (with EtOH , concentrated HCl , SnCl_2), $3\text{-H}_2\text{NC}_6\text{H}_4\text{ClO}_3$ was obtained, $m. 32^\circ$. From PhClO_3 (with concentrated H_2SO_4 , concentrated HNO_3), $3\text{-O}_2\text{-NC}_6\text{H}_4\text{ClO}_3$ was obtained, m. $49-50^\circ$. $\text{O}_2\text{NC}_6\text{H}_4\text{Ph}$ (with I and AlCl_3) gave perchlorylnitrobiphenyl. From PhOH (with I and AlCl_3), $4\text{-HOC}_6\text{H}_4\text{ClO}_3$ was obtained. From $3\text{-H}_2\text{NC}_6\text{H}_4\text{ClO}_3$ (with anhydrous ether, anhydrous HCl), the HCl salt was obtained, decomposed. From $3\text{-H}_2\text{NC}_6\text{H}_4\text{ClO}_3$ (with Ac_2O - AcOH), $3\text{-AcNH-C}_6\text{H}_4\text{ClO}_3$ was obtained, m. $136-7^\circ$ (EtOH). PhClO_3 at atmospheric pressure and 285° detonated vigorously; in liquid and in solid form it exploded when it was subjected to impact on a detonating block. $m\text{-O}_2\text{-NC}_6\text{H}_4\text{ClO}_3$, subjected to impact on a detonating block, exploded. $p\text{-O}_2\text{NC}_6\text{H}_4\text{ClO}_3$ was exploded upon detonation of blasting caps by means of an elec. detonator. $3\text{-H}_2\text{NC}_6\text{H}_4\text{ClO}_3 \cdot \text{HCl}$ (with 20% HCl , diazotized with NaNO_2 solution) gave $3\text{-O}_3\text{ClC}_6\text{H}_4\text{N} \cdot \text{-NHC}_6\text{H}_4\text{ClO}_3 \cdot 3$, which with $\beta\text{-naphthol}$ in dilute NaOH gave a dye, $3\text{-(}\beta\text{-HOC}_10\text{H}_6\text{N:N)}\text{C}_6\text{H}_4\text{ClO}_3$, dark orange crystals, m. $200-1^\circ$, $\lambda 464 \text{ m}\mu$. Wool cloth was dyed with $3\text{-(}\beta\text{-HOC}_10\text{H}_6\text{N:N)}\text{C}_6\text{H}_4\text{-ClO}_3$ to a deep orange color, which withstood prolonged exposure in the sunlight without appreciable loss of color. $4\text{-FC}_6\text{H}_4\text{ClO}_3$ with MeONa - MeOH gave $4\text{-MeOC}_6\text{H}_4\text{ClO}_3$, $n_{28D} 1.5307$. $4\text{-F-C}_6\text{H}_4\text{ClO}_3$ with HSPh - MeONa gave $4\text{-PhSC}_6\text{H}_4\text{ClO}_3$, $n_{26D} 1.5778$. From

PhClO₃ (with FeCl₃ and gaseous Cl), 4-ClC₆H₄ClO₃, was obtained, all oily liquid.

IT 90048-78-5, m-Xylene, 2,4,5-trichloro-6-perchloryl-
90151-28-3, m-Xylene, 2,4-dichloro-6-perchloryl-
(preparation of)

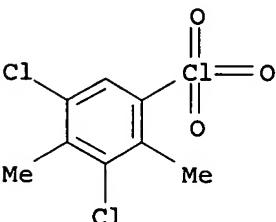
RN 90048-78-5 CAPLUS

CN m-Xylene, 2,4,5-trichloro-6-perchloryl- (7CI) (CA INDEX NAME)



RN 90151-28-3 CAPLUS

CN m-Xylene, 2,4-dichloro-6-perchloryl- (7CI) (CA INDEX NAME)



L18 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1955:45417 CAPLUS

DOCUMENT NUMBER: 49:45417

ORIGINAL REFERENCE NO.: 49:8700e-f

TITLE: Absorption spectra in relation to the chemical reactivity of some haloaromatic compounds

AUTHOR(S): Smith, F.; Turton, Lilian M.

CORPORATE SOURCE: Univ. Birmingham, UK

SOURCE: Journal of the Chemical Society (1955)

1350-4

CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

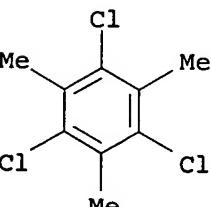
LANGUAGE: Unavailable

AB cf. J. Appl. Chemical 4, 325(1954). The ultraviolet-light-absorption spectra of a number of Cl- and F-aromatic compds. are described, and some correlation of the results with the degree of halogenation of the substances and their reactivity is attempted. The spectrophotometric measurements were carried out as previously described (cf. C.A. 45, 8352d).

IT 5324-68-5, Mesitylene, 2,4,6-trichloro-
(spectrum of)

RN 5324-68-5 CAPLUS

CN Benzene, 1,3,5-trichloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1953:11438 CAPLUS

DOCUMENT NUMBER: 47:11438

ORIGINAL REFERENCE NO.: 47:2036i,2037a-e

TITLE: Electron distribution in molecules. I. F19 nuclear magnetic shielding and substituent effects in some benzene derivatives

AUTHOR(S): Gutowsky, H. S.; McCall, D. W.; McGarvey, B. R.;

Meyer, L. H.

CORPORATE SOURCE: Univ. of Illinois, Urbana

SOURCE: Journal of the American Chemical Society (1952

), 74, 4809-17

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The effect of substituents on the electron distribution in benzene produces changes in the nuclear magnetic shielding of F atoms in the mol. A comparison of the F19 nuclear magnetic shielding in PhF with that in a substituted PhF was used in defining a δ -parameter (C.A. 46, 5433b). A radiofrequency spectroscope with slow sweep modulation was used to measure mol. differences in nuclear magnetic shielding. Exptl. δ -values were determined for the following monosubstituted PhF derivs.:

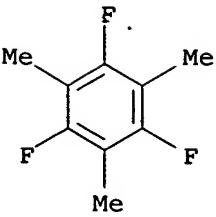
σ -, m -, and p -NO₂, -CN, -CO₂H, -I, -Br, -Cl, -F, -Me, -NHAc, -OH, -OEt, -NH₂; σ - and p -OMc; p -SO₂Cl, -CCl₃, -Ph, -OC₆H₄F, -NPh, -NMe₂; σ -CH:CHCO₂H; m -CF₃, -CH(OH)Me, -OC₆H₄F. A linear correlation was observed between Hammett's substituent constant σ and measured δ values. A least-squares solution for meta derivs. gives $\sigma_m = 1.69\delta_m$ and for para derivs., $\sigma_p = 0.560\delta_p + 0.271$.

Systematic differences in the correlation were observed and attributed to the dependence of the δ -values on the nature of the electronic interactions of the substituent. Thereby, a detailed analysis of the δ - and σ -values for particular substituents permits evaluation of the nature of their electronic effects. Consideration of σ -substituents suggests that an interaction contributes to the $\delta\sigma$ -values in some cases in addition to the usual inductive and electromeric effects at the m - and p -positions. The potential uses and limitations of $\delta\sigma$ -values in evaluating σ -effects and entropies of reaction are discussed. A determination of the extent to which substituent effects are additive was made by measuring δ -values for the following polysubstituted PhF compds. (observed F at the 1-position): 3-NO₂, 4-NH₂; 2-NO₂, 4-NH₂; 3, 5-, 2, 4-, 3, 4-, and 2, 5-di-fluoro; 3-F, 5-1; 2, 4-dinitro; 2-NH₂, 4-F; 3-NH₂, 4-F; 2-NH₂, 5-F; 3-F, 4-NH₂; 2-NO₂, 4-F; 2-NO₂, 5-F; 3-F, 4-NO₂; 2-Cl, 4-F; 3-Cl, 4-F; 2-Cl, 5-F; 3-F, 4-Cl; 2-Br, 4-F; 3-Br, 4-F; 2-I, 4-F; 3-I, 4-F; 2-I, 5-F; 3-F, 4-I; 2-CF₃, 4-F; 3-CF₃, 4-F; 2,4,6-trimethyl; 2,5-dichloro-4-F; 2, 5-dibromo-4-F; 2,4,5-trifluoro; 2, Br-4,5-difluoro; 2,4-difluoro-5-Br; 2,5-difluoro-4-Br; 2,5-difluoro-3-CF₃; 2,4-difluoro-6-CF₃; 3,4-difluoro-5-CF₃; 2,4,6-trimethyl-3-F; 2,4,6-trimethyl-3,5-difluoro. The electronic effects of substituents are usually additive, but there is significant nonadditivity between substituents in about 1/3 of the compds. studied, demonstrating interaction between substituents. A δ' parameter, analogous to δ , is defined in terms of the change produced by a substituent in the ring on the F19 nuclear magnetic shielding in benzotrifluorides. The δ' -values were determined for the following substituted benzotrifluorides: σ -, m -, and p -Cl, -CF₃; σ - and m -NH₂; m -F, -Br, -NO₂. The δ' -values are about 1/10 of the δ -values for the same substituents; this indicates the extent of attenuation of the substituent effects in the side chain.

IT 363-64-4, Mesitylene, 2,4,6-trifluoro-
(fluorine nuclear magnetic shielding in)

RN 363-64-4 CAPLUS

CN Benzene, 1,3,5-trifluoro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)



L18 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1947:8981 CAPLUS

DOCUMENT NUMBER: 41:8981

ORIGINAL REFERENCE NO.: 41:1870a-i,1871a

TITLE: Vulcanization of GR-S with halogen compounds

AUTHOR(S): Sturgis, B. M.; Baum, A. A.; Trepagnier, J. H.

CORPORATE SOURCE: E. I. du Pont de Nemours & Co., Wilmington, DE

SOURCE: Journal of Industrial and Engineering Chemistry (Washington, D. C.) (1947), 39, 64-8

CODEN: JIECAD; ISSN: 0095-9014

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

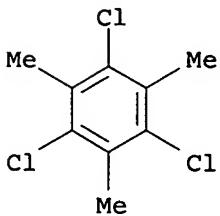
AB In a search for new types of compds. which vulcanize GR-S without S with formation of products with superior resistance to heat, a new class of vulcanizing agents was found comprising halogenated organic compds. which can in turn be divided into 3 groups: (1) chlorinated arylmethyl compds. containing at least 1 substituent Cl atom in the methyl group; (2) halogenated aliphatic hydrocarbons containing at least 1 CX3 group, where X is Cl, Br, or I; (3) aliphatic compds. containing 1 CCl3 group attached to a strong polar group. The compds. tested include benzyl chloride, 2,4-dichlorobenzyl chloride, 2,4,6-trichlorobenzyl chloride, benzal chloride, 2,6-dichlorobenzal chloride, benzotrichloride, o-chlorobenzotrichloride, 2,4-dichlorobenzotrichloride, 1-trichloromethylnaphthalene, 1,1,1,3-tetrachloropropene, 1,1,1-trichloropentane, 1,1,1-trichloroheptane, 1,1,1,9-tetrachlorononane, 1,1,1,5-tetrachloropentane, 1,1,1,5-tetrachloro-2-pentene, octachloro-1,3-pentadiene, hexachloroethane, heptachloropropene, pentachloropropene, pentachloroethane, bromoform, iodoform, C tetrabromide, telomer mixture, trichloroacetic acid, Et trichloroacetate, Zn trichloroacetate, Pb trichloroacetate, N-trichloroacetylurea, Na trichloroacetate, trichloromethanesulfochloride. All these compds. are unique in that they are primary vulcanizing agents for GR-S, yet do not vulcanize natural rubber in the absence of S. Group (1) members are, in general, the most active and they vulcanize GR-S at room temperature without any accessory agent. A large number of halogenated aromatic compds. including hexachlorobenzene, benzene hexachloride, 9,10-dichloroanthracene, 2,4,6-trichloromesitylene, benzotrifluoride, 2,4,6-trichlorobenzotrifluoride, and other analogous F compds. did not vulcanize GR-S. They are highly activated by some metal oxides, particularly PbO; e.g., with the latter vulcanizates with 2.5% of o-chlorobenzotrichloride having phys. properties close to those of S vulcanizates are obtained. The oxides tested include CeO₂, Cu₂O, CuO, Pb₃O₄, PbO₂, PbO, MgO, MgO₂, MnO₂, TeO₂, ZnO, and ZnO₂. MgCO₃, CaCO₃, and lithopone also are activators. In group (2), F compds. are inactive, and when alone the Cl and Br compds. are inactive in the absence of a metal oxide; in fact, PbO is the only highly effective oxide. The following compds. were inactive or only slightly active: 1,2,3-tribromobutane, 1,2,3,4-tetrabromobutane, 1,2,3-tribromo-2-methylpropane, 1,2,3,4-tetrachlorobutane, 1,2,3,3-tetrachlorobutane, 1,2,2,3-tetrachlorobutane, 2,2,3-tribromobutane, 1-4-dibromo-2-butene, 1,2-dibromo-1-chloroethane, 3,4-dibromohexane, 1,1,2,2-tetrabromoethane, hexachlorobutadiene, n-butyl iodide, 1,1,7-trichloroheptene, 1,3,3,4,5,6-hexachlorohexane, and methyl iodide. S retards the action of aliphatic halogenated compds. With group (3), both ZnO and S are activating agents and are necessary for the best quality of vulcanizates but they are not necessary to obtain vulcanizates of fair quality. PbO, MgO, Pb₃O₄, MoO₃, and ZnO₂ are less effective activators. That compds. of group (3) are primary vulcanizing agents with S present is evidenced by

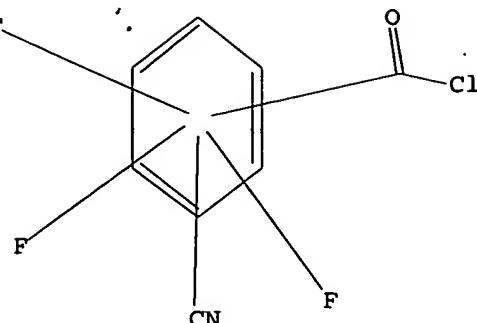
the fact that amines, e.g. tetraethylenepentamine, activate S alone but retard a combination of S and ethyl trichloroacetate. In general, the halogenated organic vulcanizing agents give GR-S vulcanizates which are characterized by particularly good resistance to elevated temps., e.g. aging at 100°. The mechanism of vulcanization by these compds. does not conform perfectly to any current theories of vulcanization by non-S compds., but the mechanism is possibly analogous to that of BzO₂ (cf. Alfrey, Hendricks, Hershey, and Mark, C.A. 39, 5542.4), i.e.: initial decomposition into free radicals; reaction of the free radicals with the polymer, with elimination of an α -methylenic H atom and formation of an odd electron; reaction of the polymer free radical with a polymer mol., probably with 1 of the double-bond electrons, with cross-linking; and continuation of the process, either by a sequence of cross-linking through the double bonds of addnl. chains or by chain transfer, until a termination reaction takes place.

IT 5324-68-5, Mesitylene, 2,4,6-trichloro-
(as vulcanizing agent in Buna-S)

RN 5324-68-5 CAPLUS

CN Benzene, 1,3,5-trichloro-2,4,6-trimethyl- (9CI) (CA INDEX NAME)





Structure attributes must be viewed using STN Express query preparation.

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REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 13:52:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 88 TO ITERATE

100.0% PROCESSED 88 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1198 TO 2322
PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

L16 0 L15

=> s 114 full

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 13:52:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1608 TO ITERATE

100.0% PROCESSED 1608 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

L17 1 SEA SSS FUL L14

L18 4 L17

=> d 1-4 ibib abs hitstr

L18 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:709043 CAPLUS